

Anti-Cancer, Anti-Osteoporosis, and Molecular Docking Studies of Novel Chalcone and Epoxy Chalcone

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Abstract: Cancer is a leading cause of death worldwide. Osteoporosis is a bone condition that causes the bones to become porous and lose density. Discovering, searching, and develop for a drug against cancer and at the same time preventing osteoporosis is very important. Chalcone and epoxy have an interest as potential drug candidates due to their easy synthesis. The present study target compounds were screened for potential anti-cancer against different cell lines (HepG2, MDA-MB-231, A549, A349, MCF-7, and HCT116) and anti-osteoporosis against cell line (MC3T3-E1). A new series of compounds evaluation by MTT assay to determine the IC₅₀, and study apoptosis and docking study. The most potent activities were the effects of the compounds CH2, CH3, and CH4 on the MDA-MB-231 cells and those of the compounds CH7 and CH9 on the HepG2. The CH7 compound proved non-cytotoxic but was antiproliferative and caused cell cycle arrest at the G0/G1 and G2/M phases. Also, the CH7, CH9, and E1 compounds displayed excellent anti-osteoporosis activity. The docking analysis showed good binding energy. The compounds CH2, CH3, and CH4 exhibited activity towards MDA-MB-231 cells and CH7 against HepG2, with induced apoptosis and cell cycle arrest, others compounds showed no significant cytotoxicity. While compounds CH7, CH9, CH9, and E1 showed good toxicity against MC3T3-E1. The molecular docking study revealed that there was evidence of good interaction and the most stable complex for inhibition.

Keywords: chalcone, epoxy chalcone; anti-cancer; anti-osteoporosis; molecular docking study.

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1. Introduction

The most public health danger is cancer which represents the second leading cause of mortality after heart diseases across the world, due to be one of the most intractable diseases due to rapid cell growth and proliferate uncontrollably, avoid apoptosis, invade metastasis[1-3]. Many studies have explored the molecular mechanism of anti-tumor effects of different compounds, which can induce dependent apoptotic cell death and regulate the expression of anti-apoptotic cells [4-6]. World Health Organization (WHO) reported new cases each year and more than 19 million people deaths in the year 2020 in world. On the other hand, lung, prostate, colorectal, stomach, and liver cancers are the most common types of cancer in men, while breast, colorectal, lung, cervical, and thyroid cancers are the most common among women[1]. Despite all years of developing drugs, cancer remains a major public health problem. Another big health problem is osteoporosis facing women and older people of both sexes. Osteoporosis is a systemic bone disease, which the bones become porous and decrease